

Nithiamide
140-40-9 | DTXSID6046391

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 259 °C

Global applicability domain: Inside

Local applicability domain index: 3.70e-01

Confidence level: 5.63e-01

Nearest Neighbors from the Training Set

Image not found

Nithiamide

Measured: 265

Predicted: 259

Image not found

Niridazole

Measured: 261

Predicted: 244

Image not found

Tenonitrozole

Measured: 256

Predicted: 234

Image not found

2-Amino-5-(5-nitro-2-furyl)-1,3,4-thiadiazole

Measured: 280

Predicted: 261

Image not found

Ethyl 2-amino-4-(trifluoromethyl)-1,3-thiazole-5-carboxylate

Measured: 187

Predicted: 180